

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 271 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.16e-01

Confidence level: 8.08e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Siduron

Measured: 204

Predicted: 210

[Image not found](#)

N-Cycloheptyl-N'-phenylurea

Measured: 234

Predicted: 218

[Image not found](#)

Isopropylpropyzamide

Measured: 148

Predicted: 173

[Image not found](#)

Pentanochlor

Measured: 575

Predicted: 365